CS 150 Quantum Computer Science

Lecture 3: Reversible circuits

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1 Overview

Last time:

- Quantum bit
- Classical digital computation

Today:

- Classical reversible circuits
- The uncertainty principle

2 Classical reversible computations

2.1 Simple Boolean gates

Now let's study a few Boolean gates

- We already saw, AND, OR, NOT, and XOR gates.
- **Question:** Is AND reversible? How about OR? How about NOT?
- SWAP
- Controlled Not operation
- Toffoli

Exercise: Prove $SWAP = CNOT_{12}CNOT_{21}CNOT_{12}$.

2.2 Universal classical computation via reversible gates

Toffoli gate: $T(x, y, z) = (x, y, (x \wedge y) \oplus z)$.

Below we show that Toffoli gate is universal for classical computation

- **AND:** a.k.a. controlled-controlled NOT $T(x, y, 0) = (x, y, x \wedge y)$
- **NOT:** $T(x, 1, 1) = (x, 1, \bar{x})$
- **OR:** $T(\bar{x}, \bar{y}, 1) = (\bar{x}, \bar{y}, NOT(\bar{x} \wedge \bar{y})) = (\bar{x}, \bar{y}, x \vee y)$
- De Morgan's Law

Fredkin gate: Controlled SWAP

$$F(x, y, z) = \begin{cases} (x, y, z) & x = 0 \\ (x, z, y) & x = 1. \end{cases}$$

Exercise: Prove the Fredkin gate is Universal.

2.3 Matrix representation of classical operations

- Let's start with a simple operation. What is the matrix representation of identity? It maps $0 \to 0$ and $1 \to 1$. It is
$$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$
- What is the matrix representation of the NOT operation?
$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$
- What is the matrix representation of a constant matrix (a matrix that always outputs 0 or 1)?
$$\begin{pmatrix} 1 & 1 \\ 0 & 0 \end{pmatrix} \quad and \quad \begin{pmatrix} 0 & 0 \\ 1 & 1 \end{pmatrix}$$
  - Note this matrix is singular
- What is the matrix representation of AND? Here is the answer.
$$\begin{pmatrix} 1 & 1 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

  But let me teach you a systematic way of finding such representations. We introduce the "bra" notation:
$$\langle 0| = \begin{pmatrix} 1 & 0 \end{pmatrix}, \quad \langle 1| = \begin{pmatrix} 0 & 1 \end{pmatrix}.$$

Using this notation, we can find the representation for AND.

$$|0\rangle(\langle 00| + \langle 10| + \langle 01|) + |1\rangle\langle 11| = \begin{pmatrix}1\\0\end{pmatrix}\begin{pmatrix}1 & 1 & 1 & 0\end{pmatrix} + \begin{pmatrix}0\\1\end{pmatrix}\begin{pmatrix}0 & 0 & 0 & 1\end{pmatrix}, \tag{1}$$

$$= \begin{pmatrix}1 & 1 & 1 & 0\\0 & 0 & 0 & 1\end{pmatrix}. \tag{2}$$

How about OR?

$$|1\rangle(\langle 10| + \langle 01| + \langle 11|) + |0\rangle\langle 00| = \begin{pmatrix}0\\1\end{pmatrix}\begin{pmatrix}0 & 1 & 1 & 1\end{pmatrix} + \begin{pmatrix}1\\0\end{pmatrix}\begin{pmatrix}1 & 0 & 0 & 0\end{pmatrix}, \tag{3}$$

$$= \begin{pmatrix}1 & 0 & 0 & 0\\0 & 1 & 1 & 1\end{pmatrix}. \tag{4}$$

How about XOR?

$$|1\rangle(\langle 10| + \langle 01|) + |0\rangle(\langle 00| + \langle 11|) = \begin{pmatrix}1\\0\end{pmatrix}\begin{pmatrix}0 & 1 & 1 & 0\end{pmatrix} + \begin{pmatrix}0\\1\end{pmatrix}\begin{pmatrix}1 & 0 & 0 & 1\end{pmatrix}, \tag{5}$$

$$= \begin{pmatrix}0 & 1 & 1 & 0\\1 & 0 & 0 & 1\end{pmatrix}. \tag{6}$$

Now let's do something more complicated SWAP

$$SWAP = \begin{pmatrix}1 & 0 & 0 & 0\\0 & 0 & 1 & 0\\0 & 1 & 0 & 0\\0 & 0 & 0 & 1\end{pmatrix}$$

CNOT

$$CNOT = \begin{pmatrix}1 & 0 & 0 & 0\\0 & 1 & 0 & 0\\0 & 0 & 0 & 1\\0 & 0 & 1 & 0\end{pmatrix}$$

We can also write the matrix form for the Toffoli gate

$$Toffoli = \begin{pmatrix}1 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\0 & 1 & 0 & 0 & 0 & 0 & 0 & 0\\0 & 0 & 1 & 0 & 0 & 0 & 0 & 0\\0 & 0 & 0 & 1 & 0 & 0 & 0 & 0\\0 & 0 & 0 & 0 & 1 & 0 & 0 & 0\\0 & 0 & 0 & 0 & 0 & 1 & 0 & 0\\0 & 0 & 0 & 0 & 0 & 0 & 0 & 1\\0 & 0 & 0 & 0 & 0 & 0 & 1 & 0\end{pmatrix}$$

Exercise: Write a matrix form for the Fredkin gate.

Remark 2.1. What do all of these matrices have in common? **Answer** sum of columns go to 1 and each entry is either 0 or 1. Equivalently, sum of squares of the columns add to 1.

Fact 2.2. *Classical reversible matrices are permutation matrices.*

3 Hadamard operation and change of basis

As we discussed last time, a quantum bit is a generalization of the probability distribution for a two-level system. It is represented by a two-dimensional complex vector $\begin{pmatrix} \alpha \\ \beta \end{pmatrix}$, for $\alpha, \beta \in \mathbb{C}$, that has unit norm $|\alpha|^2 + |\beta|^2 = 1$. A quantum bit can be implemented using various physical systems. That can be polarization of light or the number of photons in an optical mode. One important example of a quantum bit is the internal spin of an electron. Electron spin can be up or down (rotating clockwise or counter-clockwise) in any direction: top-down, left-right, front-back or any other direction. Let us denote the spin up and down states using $|0\rangle$ and $|1\rangle$, respectively. Similarly define right-spin and left-spin as $|+\rangle$ and $|-\rangle$, respectively. How are these two states of basis states related to each other?

In this section, we use heuristic reasoning to deduce how the states $|+\rangle$ and $|-\rangle$. What we will provide here is an intuitive argument. In order to give a rigorous derivation, we need to use the formalism of quantum mechanics. We start by noting that each of the basis states $\{|0\rangle, |1\rangle\}$, $\{|+\rangle, |-\rangle\}$ describe the same quantum system, i.e. the electron spin. This means $|+\rangle = \alpha|0\rangle + \beta|1\rangle$ and $|-\rangle = \gamma|0\rangle + \delta|1\rangle$. They are furthermore orthonormal basis, i.e., $\langle 1|0\rangle = \langle 0|1\rangle = 0$ and $\langle 0|0\rangle = \langle 1|1\rangle = 1$; similarly $\langle +|-\rangle = \langle -|+\rangle = 0$ and $\langle +|+\rangle = \langle -|-\rangle = 1$. $\alpha^*\delta + \beta^*\gamma = 0$, furthermore $|\alpha|^2 + |\beta|^2 = 1$ and $|\gamma|^2 + |\delta|^2 = 1$. Let's assume $\alpha, \beta, \gamma, \delta$ are all real numbers. We can show that (up to a global sign) our solution to these equations takes a form like:

$$|+\rangle = \alpha|0\rangle + \beta|1\rangle, \quad |-\rangle = \beta|0\rangle - \alpha|1\rangle,$$

Here $\alpha^2 + \beta^2 = 1$. How can we find α and β? To do this, we need to evaluate the inner product $\alpha = \langle 0|+\rangle$. We recall that $|\langle 0|+\rangle|^2$ is the probability of observing the state $|+\rangle$ to be 0. Can we design an experiment to deduce this? The Stern-Gerlach experiment, which we talked about during the first lecture, exactly performs this measurement. In the Stern-Gerlach experiment, we prepare two opposite magnets (oriented top-down) designed in a way that a spin-up electron will move upwards and a spin-down electron will move down. Please see Figure 1 (For more information you can read the Wikipadia article `https://en.wikipedia.org/wiki/Stern%E2%80%93Gerlach_experiment`). Classical physics predicts that if the orientation of the electron spin is an angle other then up or down then the electron beam should land somewhere between the top or down position at the screen (see arrow number number 4 in the Figure). Particularly, if the spin is in the left-right direction, it should not be deflected at all. The surprising outcome of the Stern-Gerlach experiment is that we only see a top point or a bottom point (see arrow number 4 in the Figure) from the experiment. That means the value of spin is quantized and once we measure it, it takes a value up or down. What is the state of the electron before measurement? It is a "superposition" of top and down. Superposition is a fundamental concept in quantum physics. What if I rotate the experimental setup 90 degrees and measure the left-right spin? Surprisingly, we get two points again. One on the leftmost side of the screen and one on the rightmost side. So, in a way, the state of each electron before measurement is in a superposition of being up or down, and at the same time, it is in a superposition of being left and right. We do not have a classical counterpart for such an observation.

The electron beam in this experiment is in a highly complex mixture of spins in various directions. What if we do an experiment to make sure all electron beams are in the top direction? See Figure 3. We compose two Stern-Gerlach (SG) experiments. In the first experiment we compose two top-down experiments. We see that in the first experiment, electrons in top directions are selected, and as we pass the resulting beam through the second experiment, we only see spin-up electrons. We don't see spin-down electrons! This is consistent with our intuition. In a way, the beam going through the second experiment is deterministically in the $|0\rangle$ state. What if we pass this second beam through a left-right experiment? This is the subject of the second experiment in Figure 3. Classically, we expect that the beam should not be deflected at all. This is because the electron spin has 90 90-degree angle from the N-S magnet in the second SG experiment. To our surprise, we see that we obtain both left spins and right spins, with probability $1/2$ each. (The third experiment is very similar to the second experiment; we only exchange the order of the two SG measurements). From this experimental observation, we deduce that when the electron is in a spin-up state, it has a $1/2$ probability of being measured in spin-left or spin-right states! We hence deduce that $|\langle 0|+\rangle|^2 = \frac{1}{2} = \alpha^2$. Therefore $\alpha = \beta = \frac{1}{\sqrt{2}}$.

The uncertainty principle: Using the SG experiment (second or third experiments in Figure 3), we arrive at one of the most important concepts in quantum physics: the uncertainty principle.

> "If the electron spin is fully deterministically in the up direction, its spin value in the left-right direction is completely uncertain. If we measure the spin in the left-right direction, half of the time, we observe spin left, and the other half of the time, we observe spin right! Similarly, if we prepare an electron spin in the right-spin direction and measure the spin in the top-down direction, we get a completely uncertain outcome. Half of the time, we obtain spin up, and the other half, we obtain spin down."

In this situation, we say that the top-down and left-right spins are incompatible observables. There are several other examples of incompatible observables in quantum physics. One of the first examples of the uncertainty principle was the uncertainty principle was about the position and velocity of particles. That means if we learn the position of a particle with high accuracy, we lose the information about the velocity and vice-versa. Heisenberg explained this phenomenon using the following intuition. If we want to measure the position of a particle. We have to interact with it using, say, a photon. If we want to learn the position with high accuracy, we will have to alter the information about velocity. So we can't learn both.

Remark 3.1. This situation is similar to the uncertainty of variables that are Fourier transform of each other in signal processing and Fourier analysis. This is not a coincidence. You can read

Figure 1: The Stern-Gerlach experiment. Arrow number 4 is the classical prediction. Arrow number 5 is the actual outcome of the quantum experiment. Image Source Wikipedia.

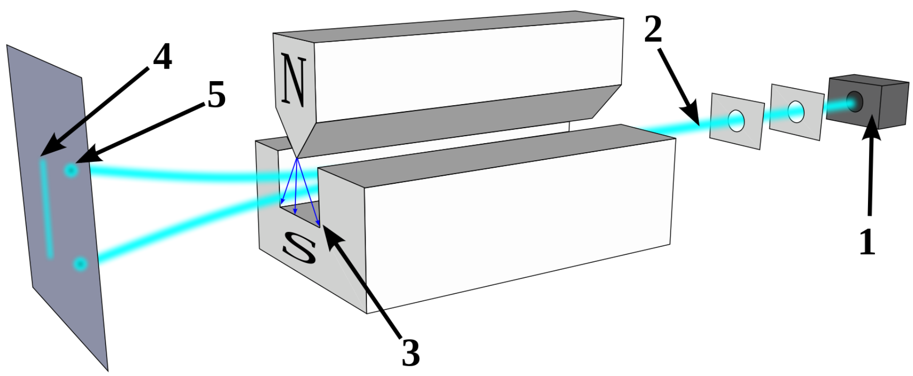
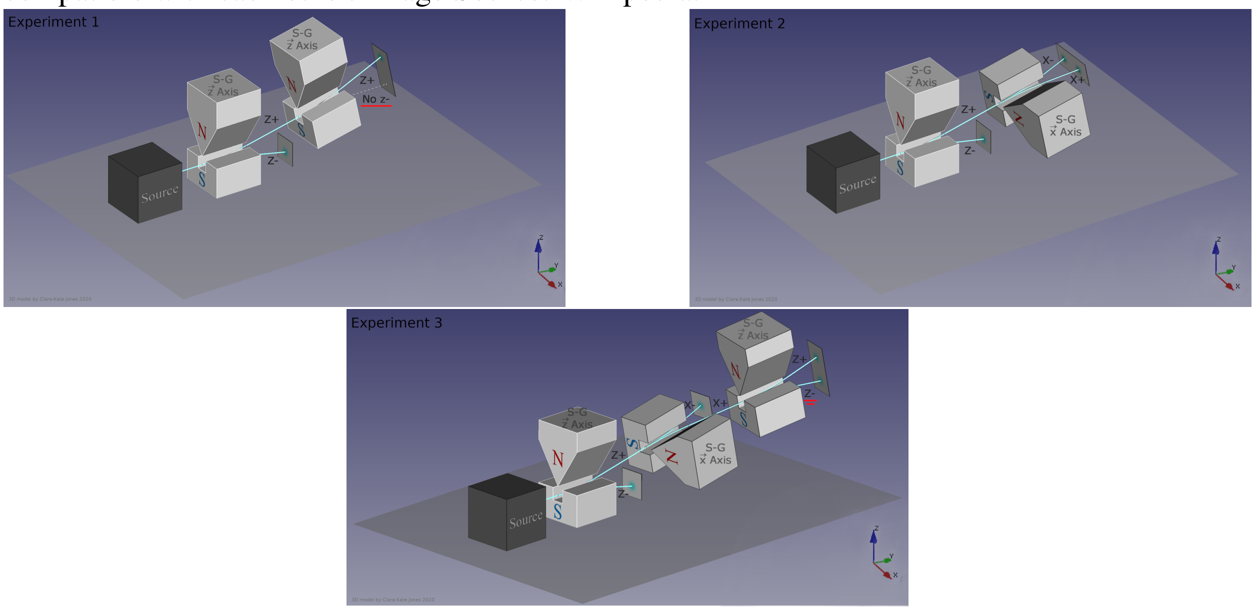


Figure 2: Three Stern-Gerlach experiments. In the first experiment we measure the top-down direction twice. In the second experiment we first measure top-down then left-right, and in the third experiment we measure left-right then top-down. While in the first experiment the outcome is deterministically a top spin in the other two experiments the outcome is probabilistic mixture of each direction. In other words, the left-right measurement and the top-down measurements are not compatible with each other. Image Source: Wikipedia.



more about the role of the Fourier transform for quantum observables in standard quantum physics textbooks. We won't delve deeper into this notion in this course.